Nonlinear Characterization of Observation Errors

Applications to Assimilation of Clouds and Precipitation

Derek J. Posselt

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Outline

1. Assimilation of clouds and precipitation: background and challenges
2. Role of observation uncertainty and the Gaussian assumption
3. Characterization of non-Gaussian observation errors
4. Examples from two well-known passive remote sensing problems
5. Implications for assimilation of clouds and precipitation

Background

- 100-fold increase in satellite data in the past decade
- 10^5 increase in the coming decade
- Key role of remotely-sensed data in modern assimilation systems—especially in the southern hemisphere
- Motivation for assimilation of clouds and precipitation
  - Predict hydrologic cycle with increased accuracy
  - Assess cloud response to and effects on climate change
  - Increase accuracy of long term prediction—clouds feed back to thermodynamic state of the atmosphere through radiation and latent heating

Cloud and Precipitation Assimilation: Challenges

- Spatial and temporal variability of clouds
- Computational limitations require simple cloud and precipitation parameterizations
- Range of spatial scales of clouds (meters to planetary)
- Difficulty of establishing metrics for success
- Forward models that link measurements to state variables are complex
- Effective assimilation of cloud and precipitation information requires in-depth knowledge of observation uncertainty

Data Assimilation: An Optimization Problem

- Combine available information to obtain an estimate $\mathbf{x}$
  1. Observations $\mathbf{y}$
  2. Relationship between observations and state $\mathbf{y}=F(\mathbf{x})$
  3. Physical nature of the system
  4. Prior knowledge of the state of the system $\mathbf{x_a}$
- Each piece of information represented as a probability distribution

$$P\left(\mathbf{x}|\mathbf{y}, F(\mathbf{x})\right)$$

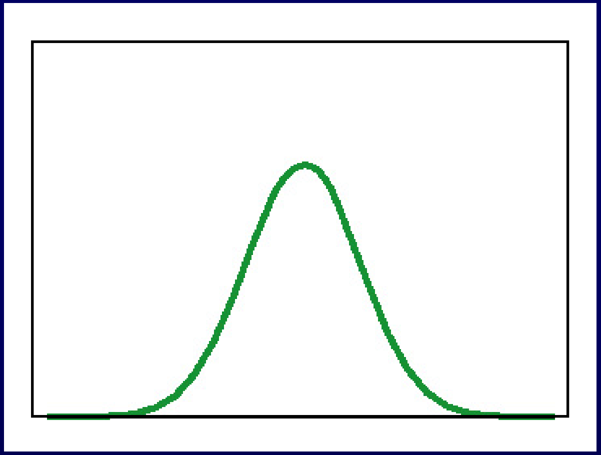
- Goal: maximize probability that state = true state *conditioned* on above information

$$P(\mathbf{x}|\mathbf{y}) = \frac{P(\mathbf{y}|\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$

Assumption: Gaussian Probabilities

- Estimation of $\mathrm{P}(\mathbf{x}|\mathbf{y})$ requires specification of the form of each probability distribution
- Gaussian (Normal) is the most straightforward
  - Defined by two moments: mean and (co)variance
  - Solution is easily reformulated as the minimum squared obs-state difference

$$P(\mathbf{x}|\mathbf{y}) = \frac{P(\mathbf{y}|\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$



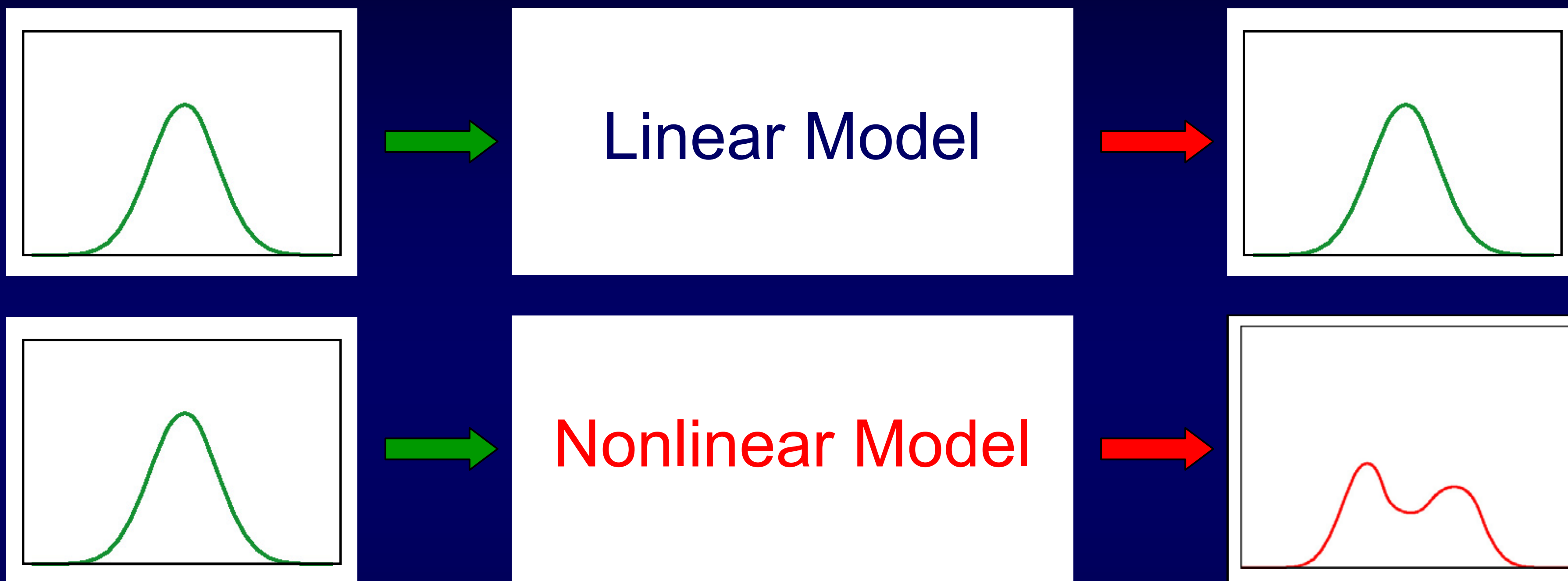
Observation Uncertainty

- Ability of observations to constrain the solution depends on correct representation of their uncertainty
- Observation uncertainty is a combination of
  - **Measurement uncertainty**
  - **Uncertainty in forward model**
  - **Representativeness error**

$$P\left(\mathbf{y}, F(\mathbf{x})|\mathbf{x}\right)$$

- Measurement uncertainty can usually safely be assumed to be Gaussian in form
- *Nonlinear* forward models produce a *non*-Gaussian probability distribution for model uncertainty

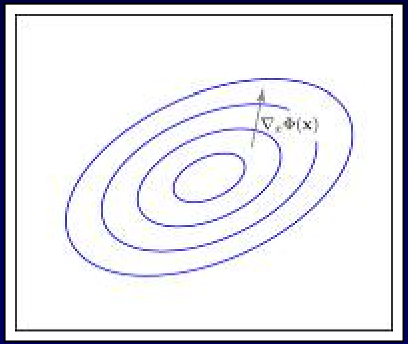
Error Assumptions

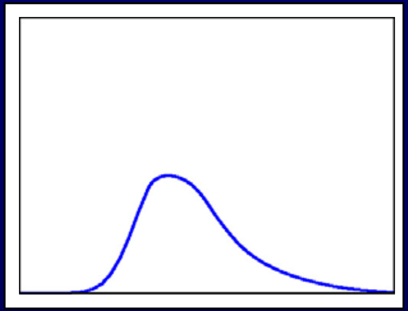


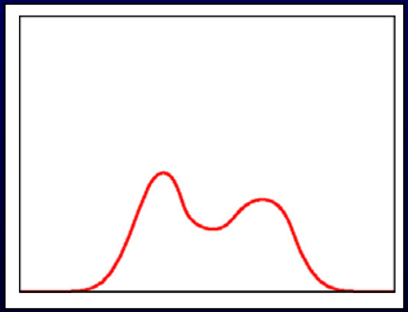
- Forward model must be linear for uncertainty to be Gaussian
- In the case of a nonlinear forward model, need to characterize actual distribution
  - Magnitude of observation error
  - Departure from Gaussian form

Characterizing the PDF

- Key information
  - Shape (correlation, skewness)
  - Number of modes (nonunique solution)
- Implications
  - **Correlation**—underlying relationship between parameters
  - **Skewness**—one set of values is favored over another
  - **Multiple modes**—model produces two sets of solutions with very similar probability
- How to characterize the PDF
  - PDF mapping
  - Sampling



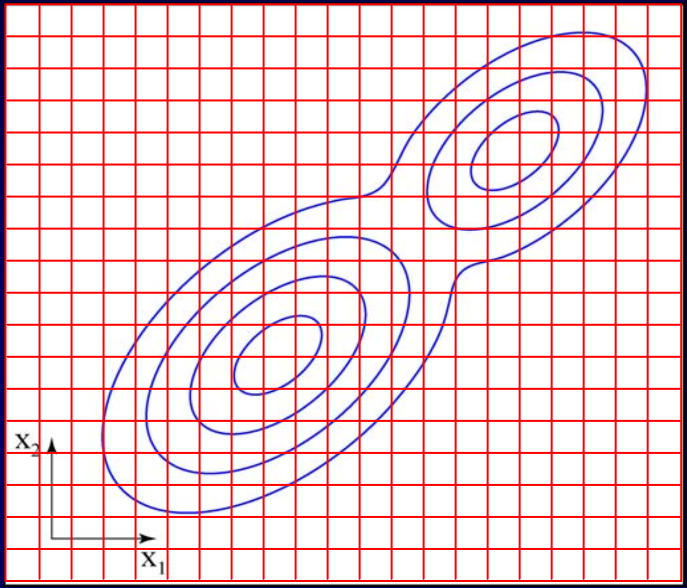




Characterizing the PDF

Two options

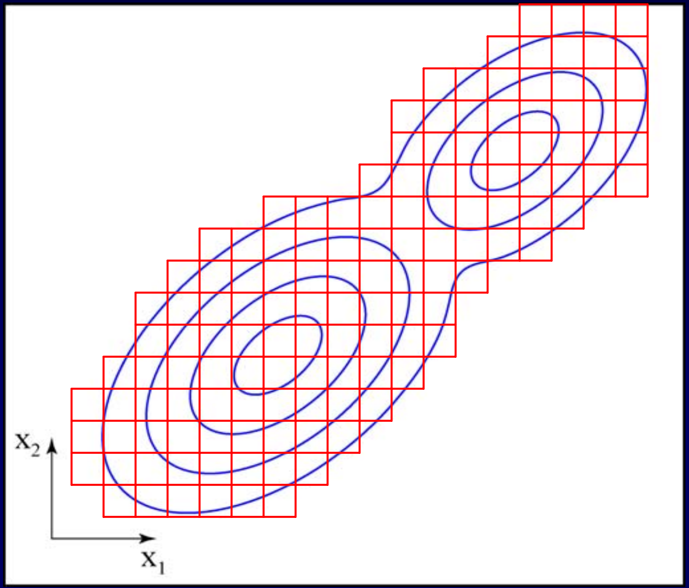
1. Exhaustive search: run the forward model over the realistic range of each parameter in small increments



Characterizing the PDF

Two options

1. Exhaustive search: run the forward model over the realistic range of each parameter in small increments **or**
2. *Sample* the PDF:
   - Seek sets of parameters that produce model states that are close to observations
   - Avoid parameters that lead to states that are very different from observations

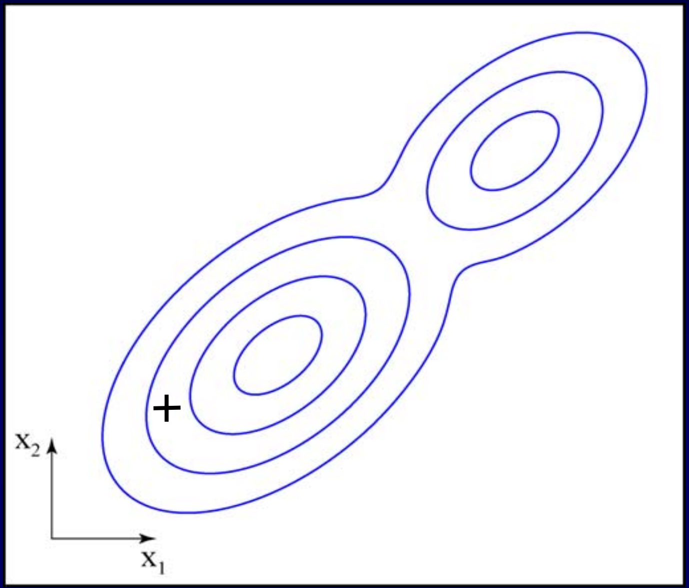


- Computational benefit of sampling increases exponentially with the number of parameters

PDF Sampling:
Markov Chain Monte Carlo

MCMC samples the conditional probability distribution

1. Randomly choose new parameter values
2. Run the forward model using the new parameter values
3. Compare the solution to observations
4. Accept the new set of parameters as a sample of the PDF if:



PDF Sampling: Markov Chain Monte Carlo

MCMC samples the conditional probability distribution

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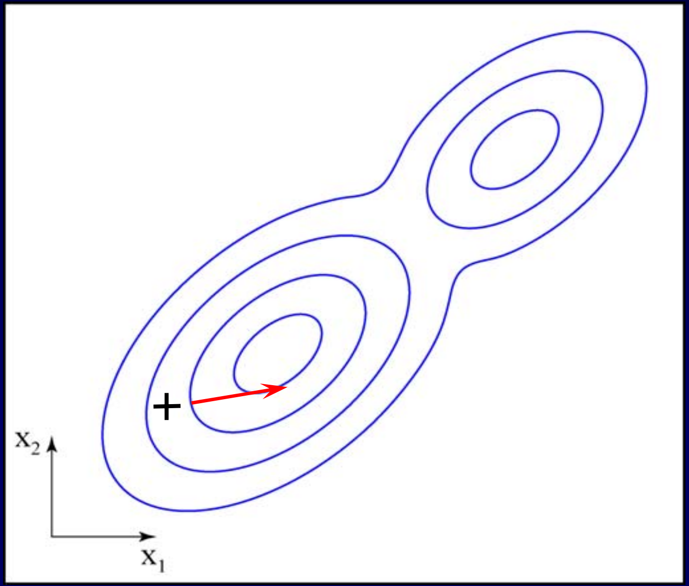
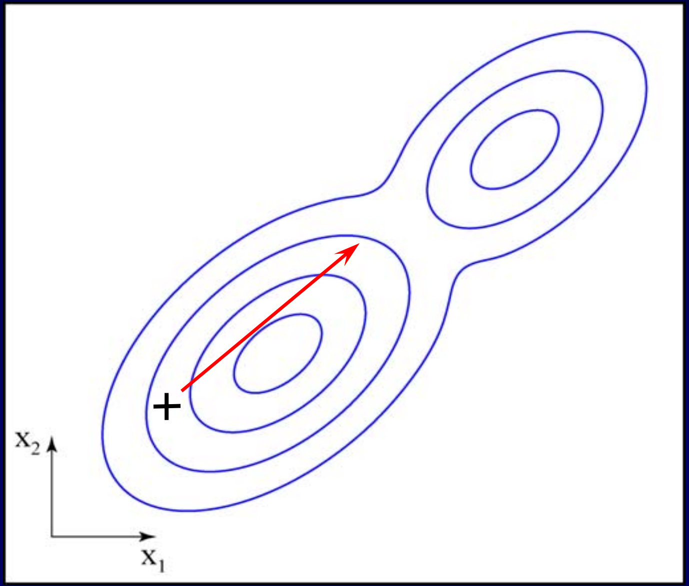
   - The new state provides a better fit to observations or



PDF Sampling: Markov Chain Monte Carlo



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PDF Sampling:
Markov Chain Monte Carlo

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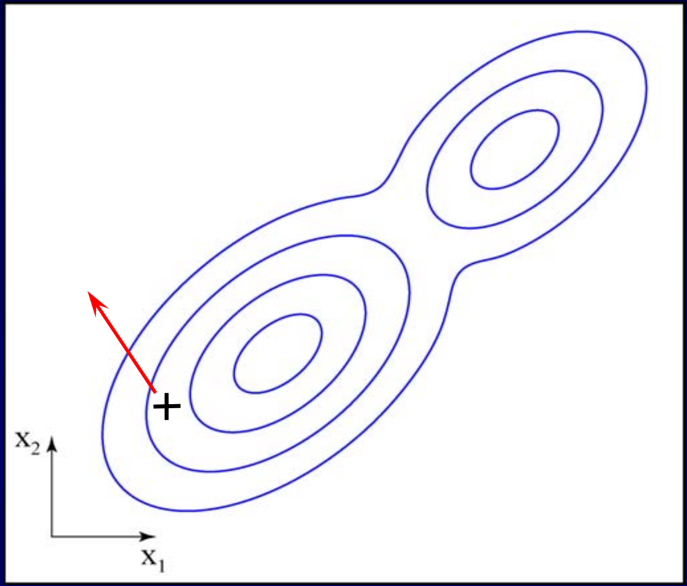
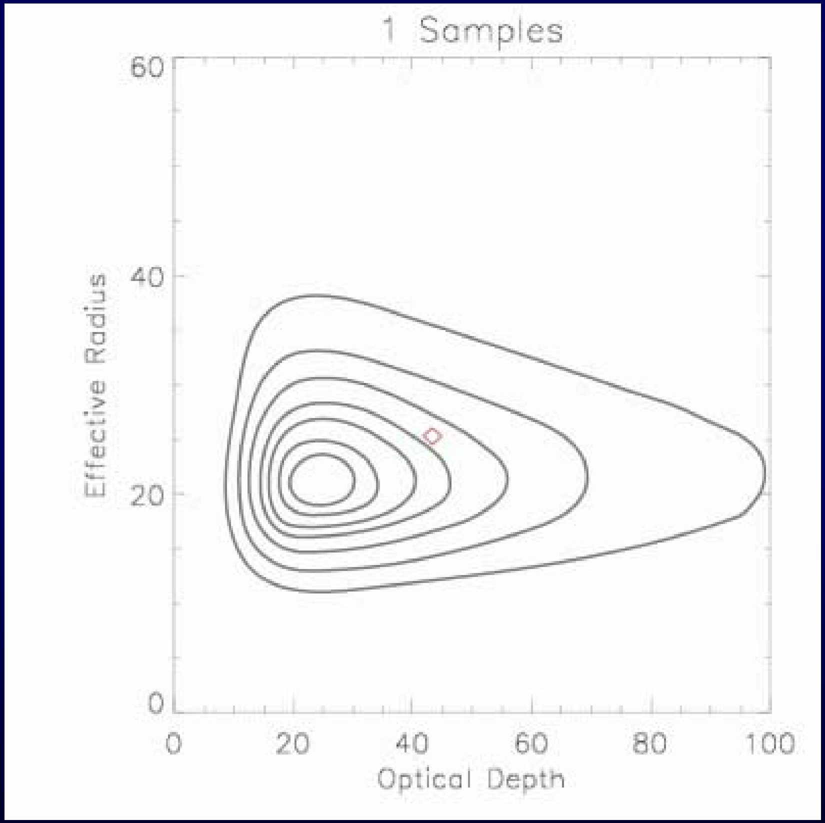


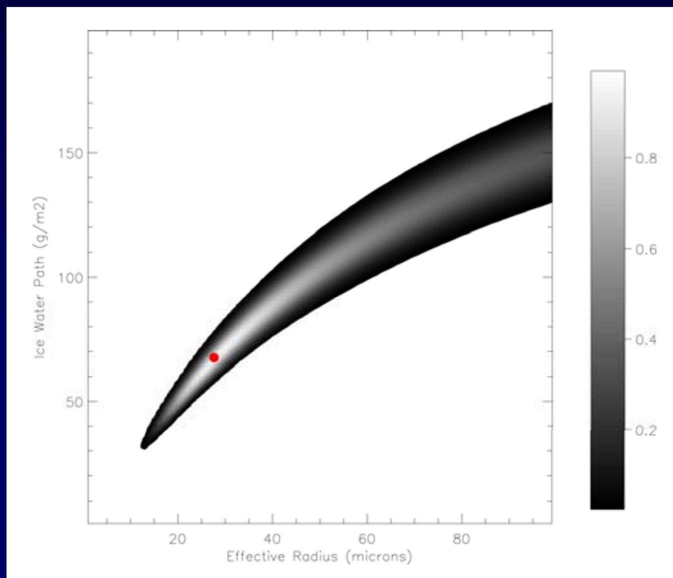
1. Randomly choose new parameter values
2. Run the forward model using the new parameter values
3. Compare the solution to observations
4. Accept the new set of parameters as a sample of the PDF if:
   - The new state provides a better fit to observations or
   - The new state provides a comparable fit to the old
5. Otherwise, reject the new set of parameters and perturb again from the old values

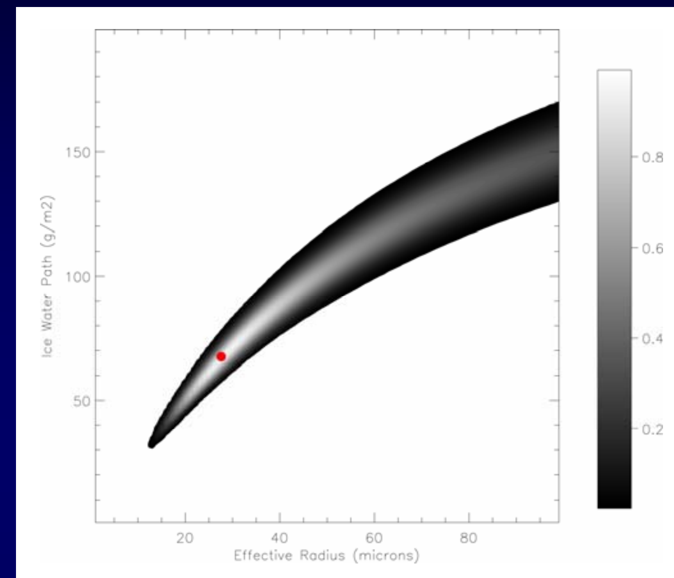
PDF Sampling: Markov Chain Monte Carlo

- Iteratively builds a sample of the underlying joint PDF



Example: PDF Map vs. MCMC





- 10x fewer iterations were required for MCMC to produce the same image—result of algorithm not venturing into space with very low probability
- Efficiency increases exponentially with dimension of the problem

Retrievals As Examples

- No numerical forecast model (or model error)
- Background errors more easily dealt with
- Focus on two commonly used cloud property retrieval techniques
  - Visible and near-infrared reflectance (Nakajima and King-type retrieval)
  - Infrared brightness temperatures (split window retrieval)
- Both provide an estimate of cloud properties
- Underlying physics differs—leads to different probability structures and different sources of error

Cloud Properties I: Visible/Near Infrared Reflectance

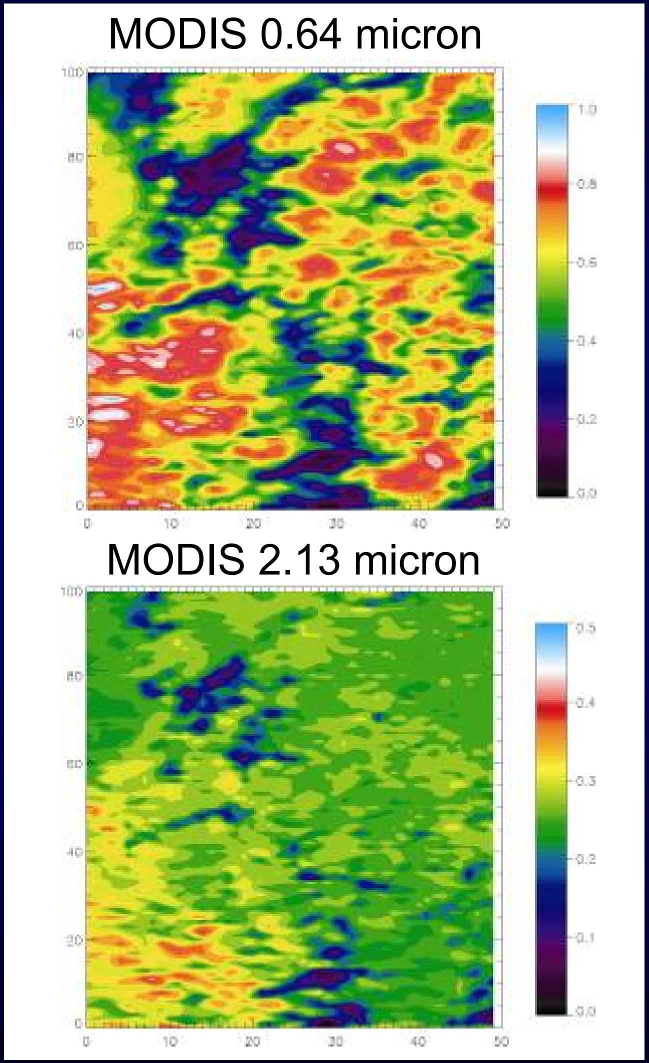
- Visible (0.64 micron) and near-infrared (2.13 micron) reflectances serve as observations
- Related to optical depth and effective radius, respectively
- Forward model: nonlinear diffuse-scattering radiative transfer model

$$\mathbf{I}(\tau) = \exp\{\mathbf{A}\tau\}\,\mathbf{I}(0)$$

- Exponential in both optical depth and effective radius (derived from single scatter albedo)
- Two observations, two unknowns—a well-constrained problem

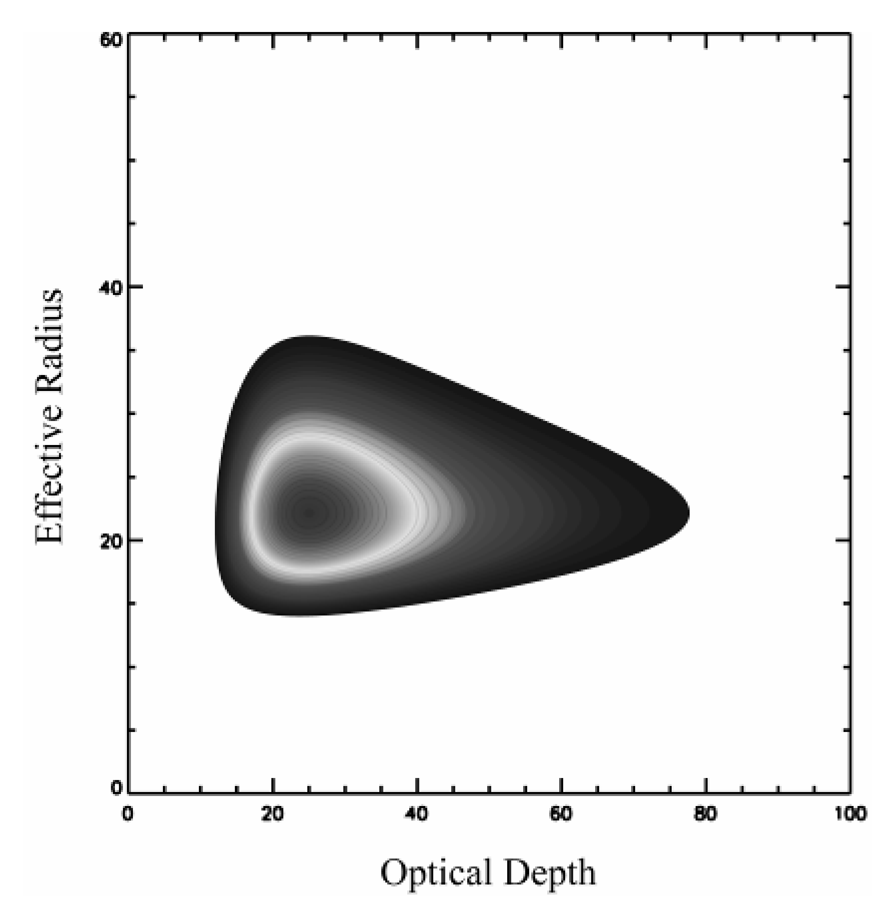
Observations

- Subset of a Terra MODIS scene
- Low broken stratus and stratocumulus over the northeast Pacific Ocean
- Observations: visible and near infrared reflectance
- State: optical depth and effective particle radius



Probability Distribution: Single Pixel

- PDF map reflects nature of forward model
- Exponential form leads to log-normal PDF in both optical depth and effective radius
- Skewness is larger for optical depth than for effective radius
- Expect Gaussian assumption to have more effect on optical depth estimate



Effect of Nonlinearity: Least Squares Retrieval

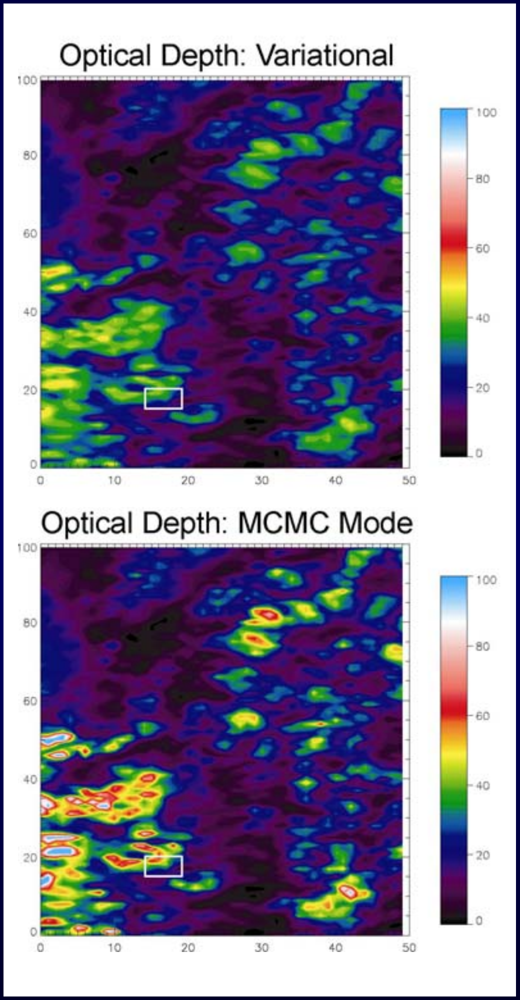
- Formulate retrieval in least-squares framework as cost function minimization

$$\Phi(\mathbf{x},\mathbf{y}) = \left[\mathbf{y}_{\mathbf{obs}} - F(\mathbf{x})\right]^T \mathbf{R}^{-1} \left[\mathbf{y}_{\mathbf{obs}} - F(\mathbf{x})\right] + \left[\mathbf{x} - \mathbf{x}_{\mathbf{a}}\right]^T \mathbf{B}^{-1} \left[\mathbf{x} - \mathbf{x}_{\mathbf{a}}\right]$$

- Compare retrieved Gaussian PDF with PDF sampled from MCMC
- Assess effect of nonlinearity on the estimate
- Focus on optical depth—higher degree of nonlinearity

Effect of Nonlinearity: Bias

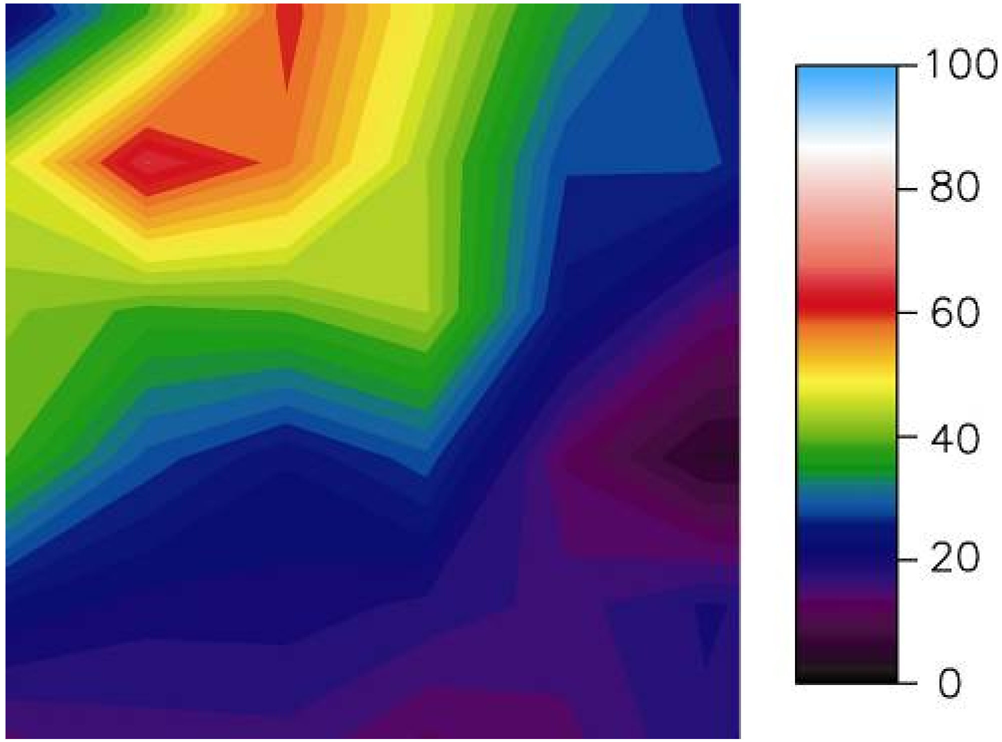
- Least squares retrieval *underestimates* large optical depth values compared with MCMC



Effect of Nonlinearity: Bias

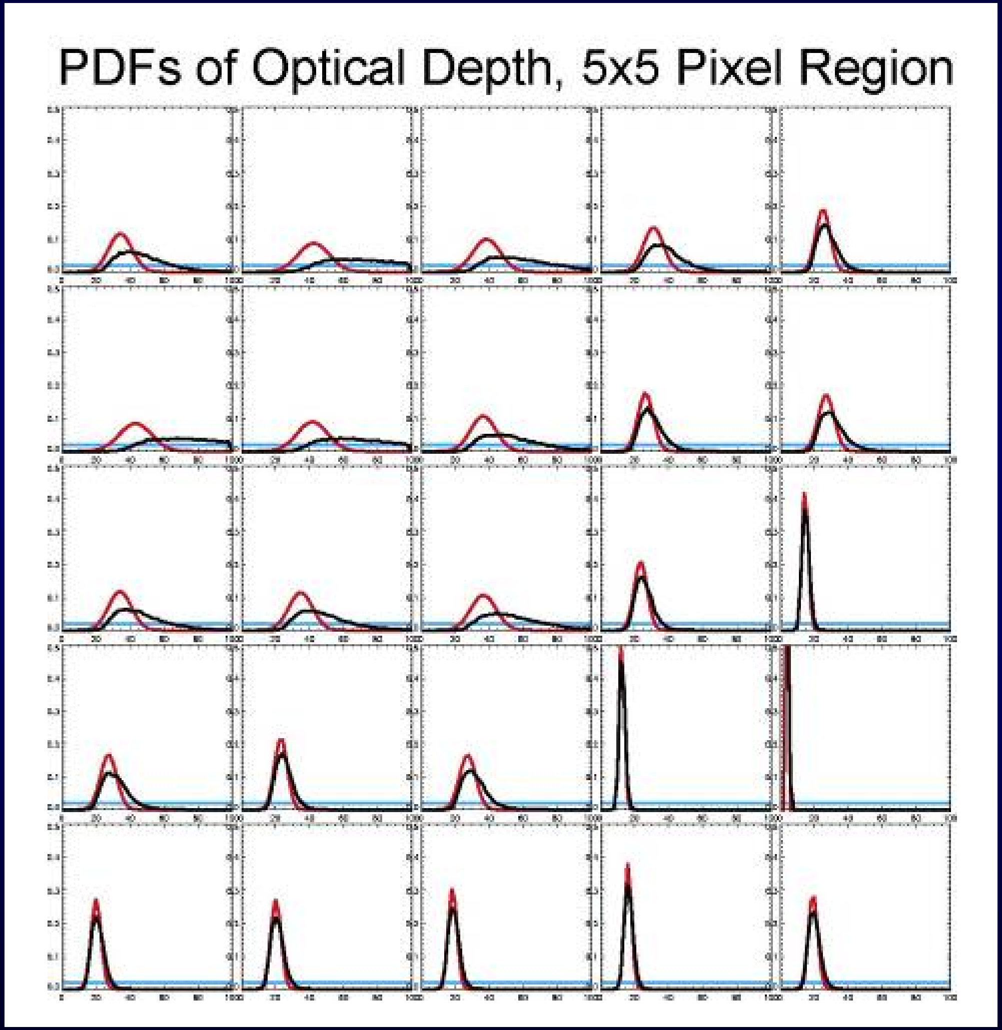
- Least squares retrieval *underestimates* large optical depth values compared with MCMC
- Compare MCMC PDFs with least squares PDFs for selected pixels to understand why

Optical Depth in
Selected 5x5 Pixel Region



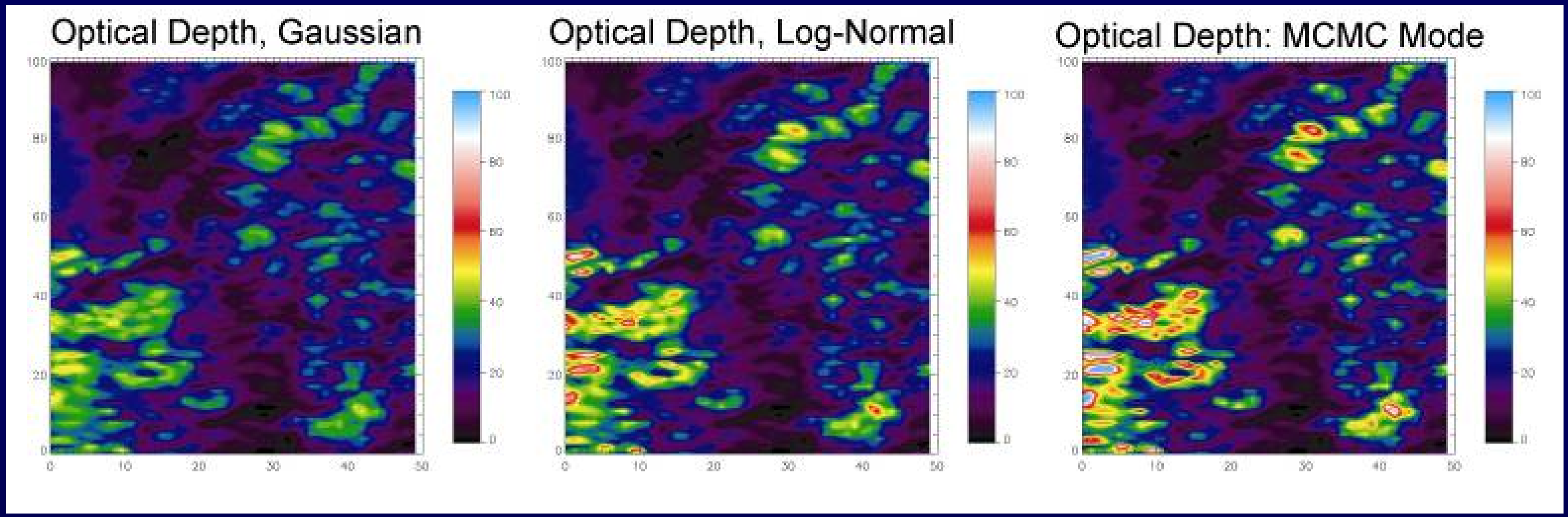
Effect of Nonlinearity: Bias

- As in single pixel estimate, PDFs of optical depth are log-normal
- Solution is well-constrained for low optical depths; large information content in the observations
- At optical depths > 50, solution collapses to uniform distribution; small information content



Solution: Variable Transform

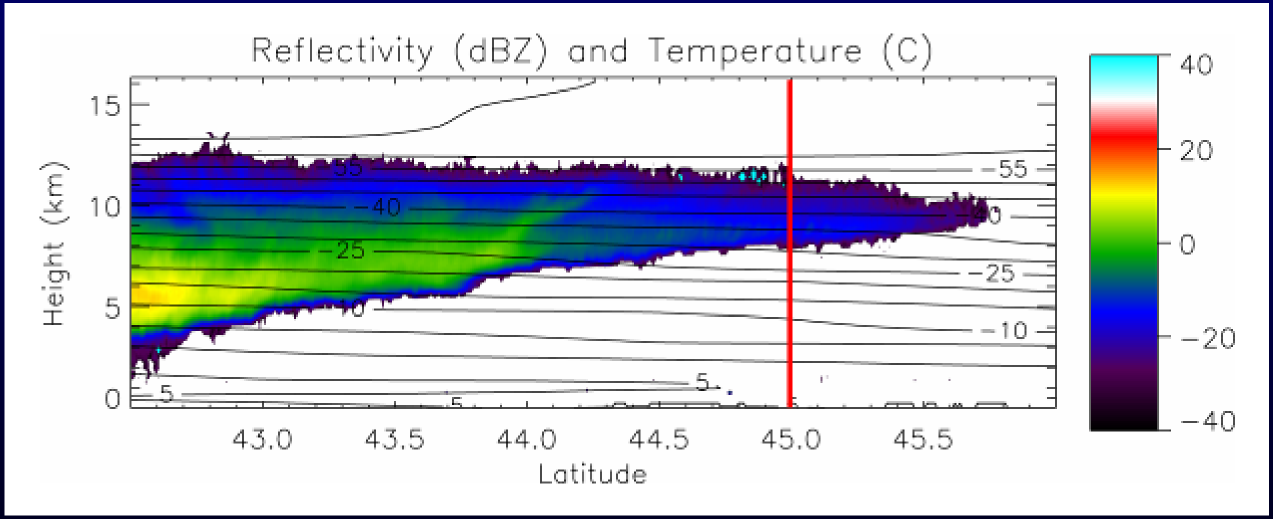
- Retrieve the natural log of the optical depth
- Increased sensitivity to large optical depths, sensitivity to low values is retained



- Implications: least squares yields an acceptable result even for a nonlinear forward model **if**
  - Observation information content is large relative to the error
  - Nonlinearity does not produce multiple modes

Cloud Properties II: Split Window

- Observations: brightness temperature at 10.8 and 12 micron infrared wavelengths
- State: ice water path (function of optical depth) and effective radius (function of single scatter albedo)
- Well-constrained problem: 2 unknowns, 2 measurements
- Scene: Warm Front over West Atlantic Ocean

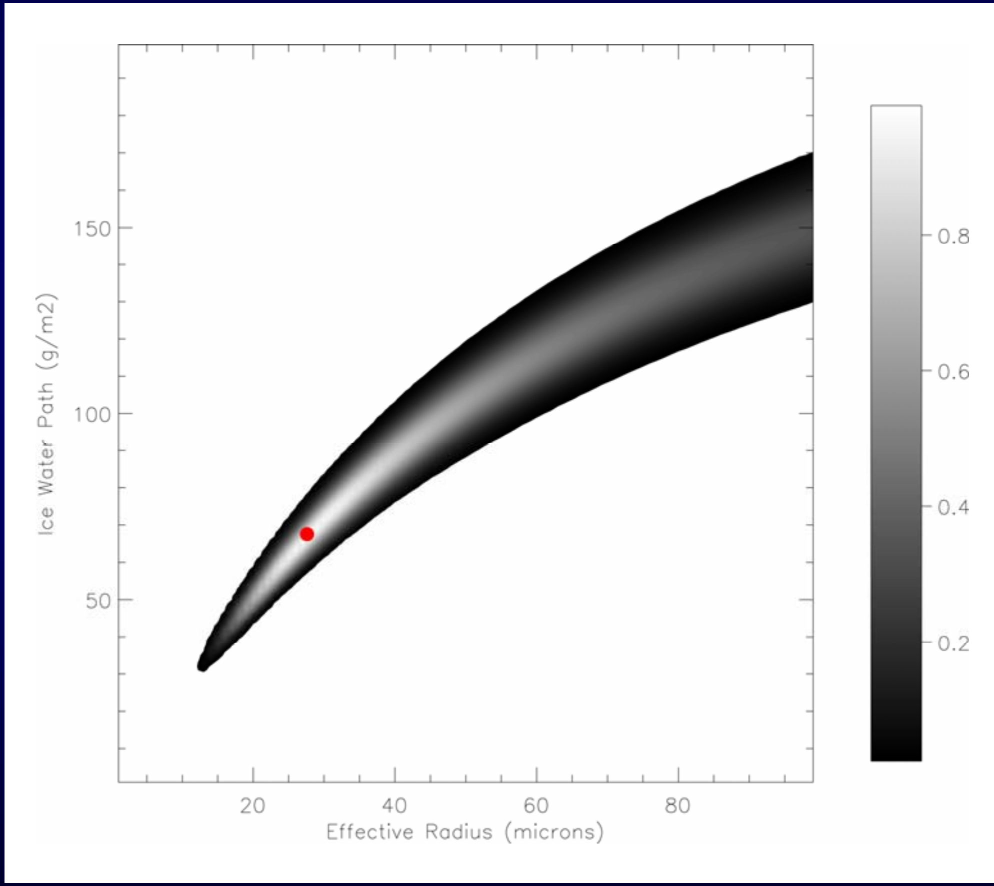


Forward Model and Background Fields

- Two physical processes to be modeled
  - Gaseous absorption: OPTRAN
  - Scattering and absorption by clouds: Successive Order of Interaction (SOI) model
- Skin temperature and temperature, water vapor, and ozone profiles from CloudSat data stream
- Cloud top height and geometric thickness from CloudSat reflectivity (uncertainty of +/- 500 meters)
- Forward model is weakly nonlinear in both optical depth and effective radius (depends on cloud thickness)

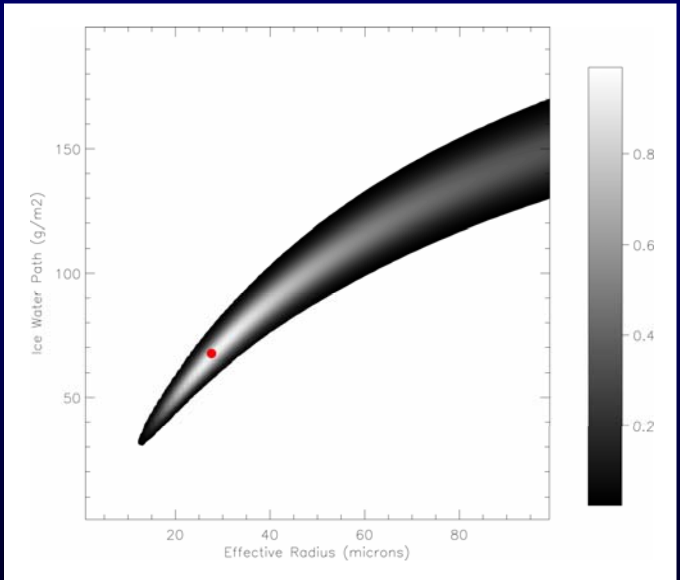
Split Window PDF

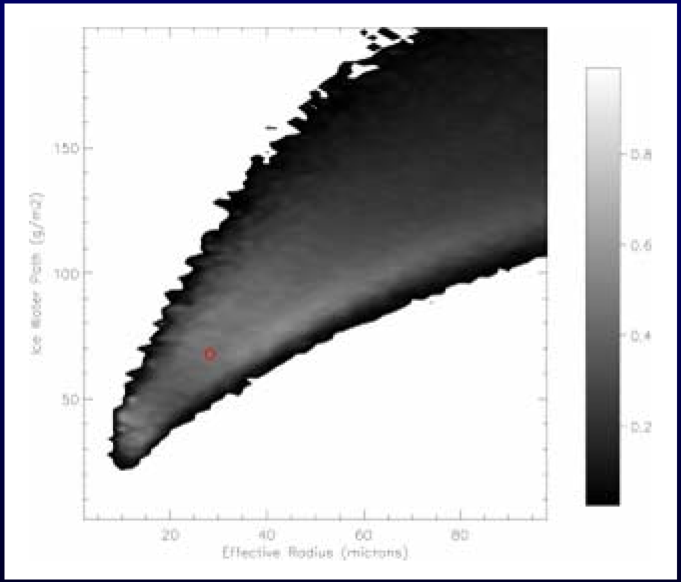
- Effective radius and ice water path are correlated
- Nonlinearity evident in skewness along correlation, as well as in curvature of relationship
- Well-defined mode, given:
  - Skin temperature
  - Cloud top temperature
  - Cloud thickness
  - Crystal shape



Split Window: Additional Sources of Error

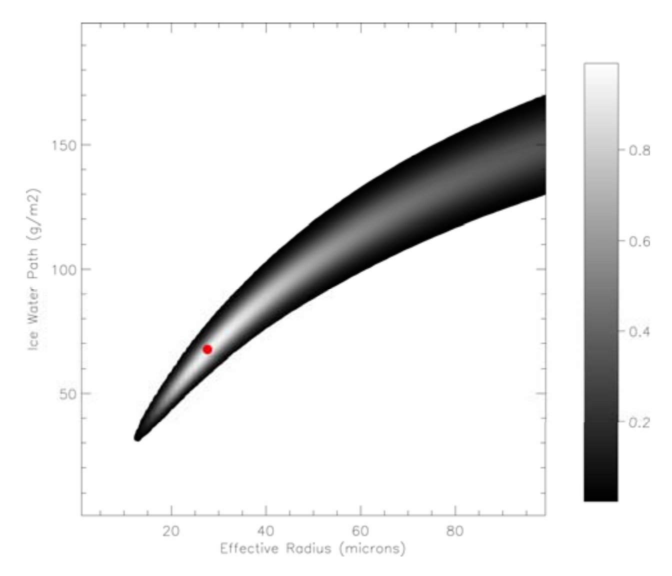
- Well-known errors associated with cloud top height, geometric thickness, ice crystal shape
- MCMC allows examination of each source of error
- Divide error sources and examine each individually

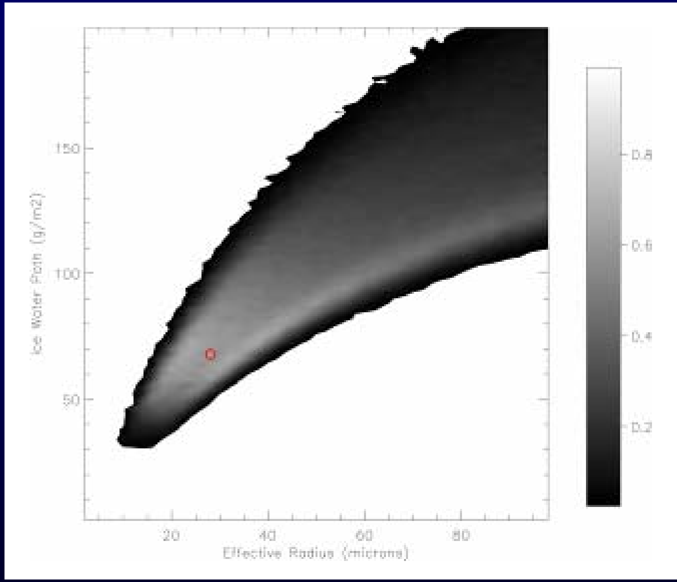




Split Window Errors: Cloud Top Height

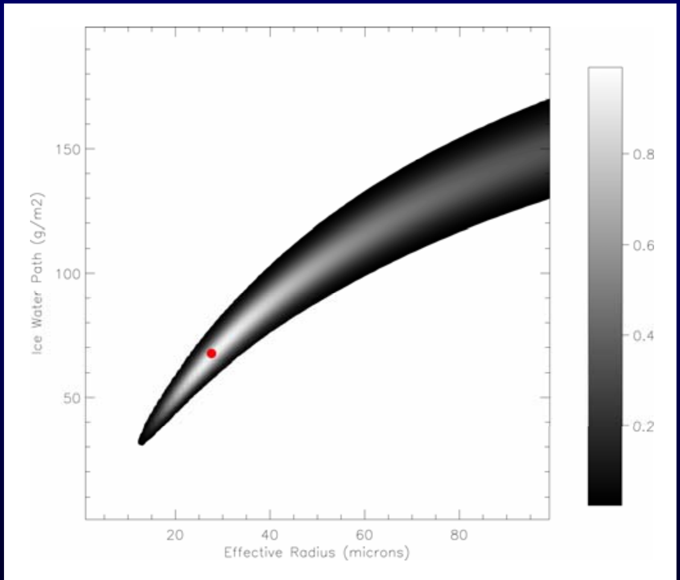
- Range of cloud top height: +/- 2 km (~ +/- 8 K)
- Errors in cloud top height contribute most of the error
- Bimodal structure evident—note that neither lies along the axis of the true mode

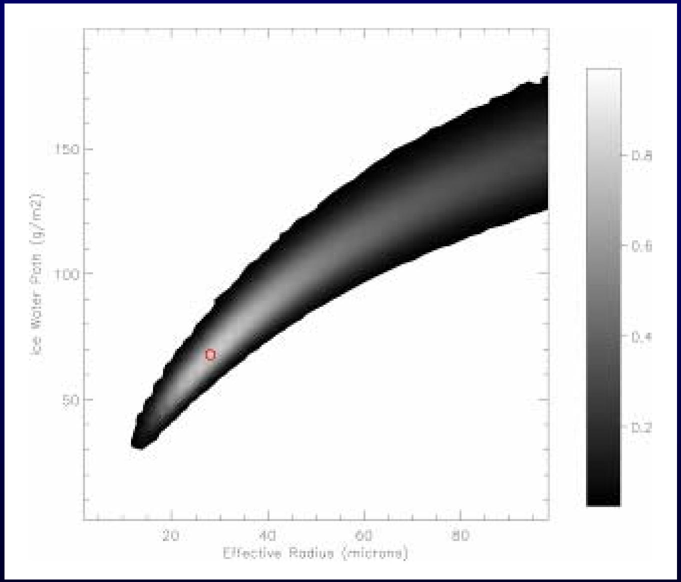




Split Window Errors: Cloud Geometric Thickness

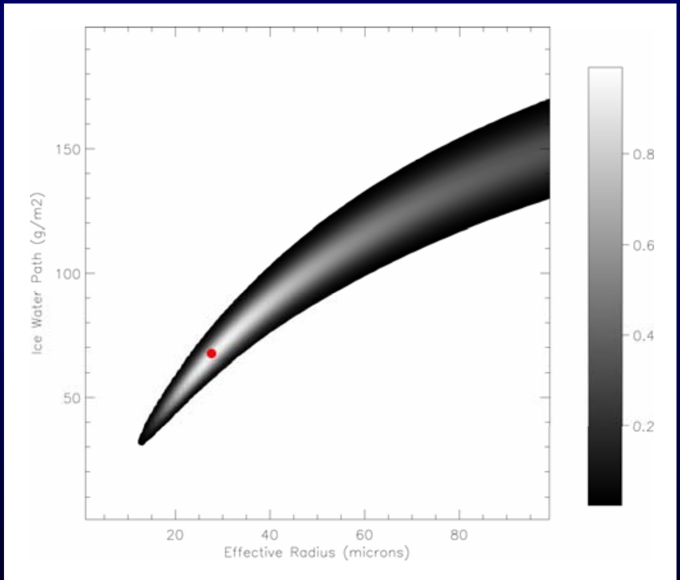
- Range of geometric thickness: +/- 2 km
- Geometric thickness variations contribute a moderate amount of error
- PDF width increases over entire range of IWP and effective radius

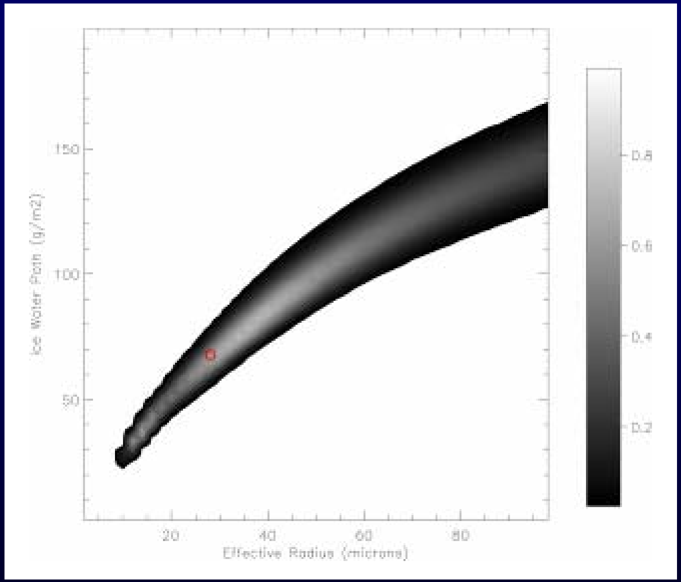




Split Window Errors: Crystal Shape

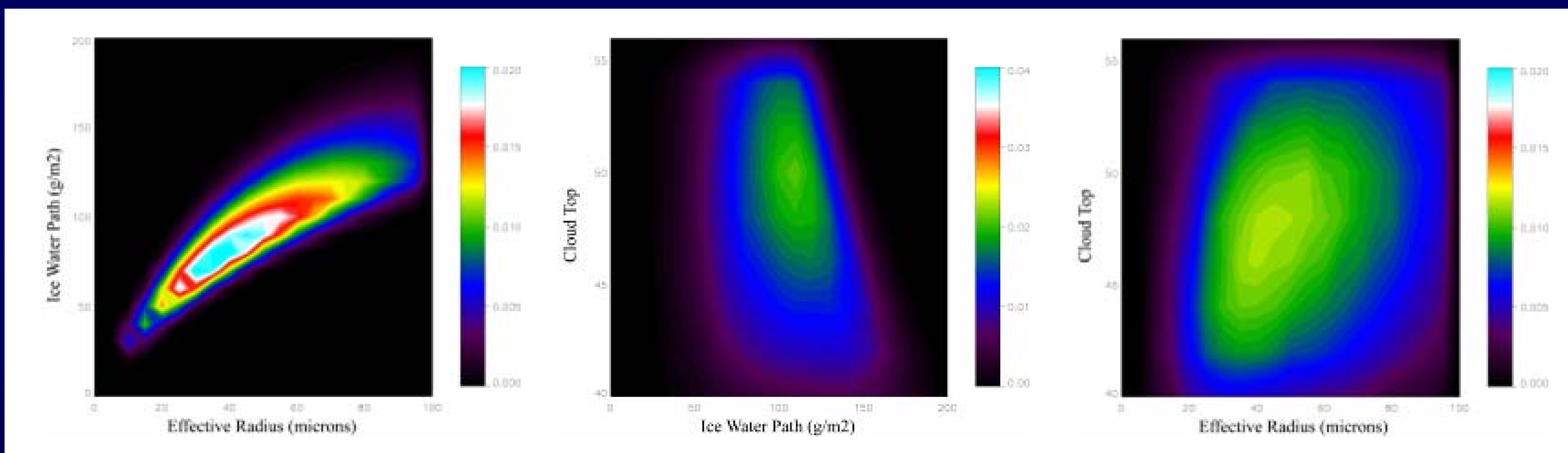
- Three crystal shapes: columns, aggregates, droxtals
- Uncertainty in crystal shape leads to broadening *along* the axis of correlation
- Secondary mode is evident at low effective radius/IWP





Error Correlations

- MCMC samples the full joint PDF of all uncertain quantities
- Any metrics can be computed from the sample
- Relationships between variables can be clearly seen



- Effective radius and ice water path are strongly related and nearly linearly correlated
- Cloud top height correlates with both ice water path and effective radius
- Effective radius and ice water path both exhibit skewness

Implications for Cloud and Precipitation Assimilation

- Modern data assimilation techniques assume linear (or nearly linear) forward model
  - Requirement of minimization
  - Tangent linear and adjoint model
- Assimilation of cloud properties from passive instruments
  - Simple relationship between radiances and cloud properties
  - In absence of forward model error, nonlinearity is not large in region of maximum likelihood
  - Variable transform can eliminate effect of nonlinearity

Implications for Cloud and Precipitation Assimilation

- Effect of forward model error
  - Visible/Near-Infrared: multiple possible solutions in ice cloud case due to different crystal shapes
  - Split window: multiple possible solutions result from cloud top temperature uncertainty and different crystal shape
- Solution: add information to reduce uncertainty
  - Additional channels to characterize liquid vs. ice
  - LIDAR/radar estimates of cloud top height and thickness
  - Physical nature of the system can be used to approximate particle shape (e.g., temperature-crystal shape relationships)

Summary

- Effective assimilation of observations depends on correct specification of observation uncertainty
- Uncertainty is a combination of forward model and measurement
- Nonlinear forward models produce non-Gaussian probability distributions
- PDF mapping can be used to characterize PDFs, but is inefficient
- Markov chain Monte Carlo methods provide a robust and efficient method for sampling the full joint observation PDF

Key Questions

- Impact of assimilation of cloud properties?
- Need for assimilation of cloud/precipitation statistics?
- How to best utilize cloud profile observations (CloudSat, TRMM, NEXRAD)?
  - Cloud boundaries?
  - Variation in cloud content with height?
- Quantitative metrics for evaluating simulations of clouds and precipitation?
  - Situation dependent?
  - Related to the public good

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